

Methyl beta-alanate
4138-35-6 | DTXSID50194322

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -1.72

Global applicability domain: Inside

Local applicability domain index: 5.58e-01

Confidence level: 4.73e-01

Nearest Neighbors from the Training Set

[Image not found](#)

N-Methylglycine

Measured: -2.78

Predicted: -2.19

[Image not found](#)

3-Aminopropanol

Measured: -1.12

Predicted: -1.28

[Image not found](#)

Diethanolamine

Measured: -1.43

Predicted: -1.46

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Butanoic acid, 4-hydroxy-, methyl ester

Measured: -0.0600

Predicted: 7.93e-02